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APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
09/502,133	02/11/2000	Harold E. Helson	103544.127	4787
7590 Jason A. Reyes Hale and Dorr LLP 60 State Street Boston, MA 02109			EXAMINER JONES, HUGH M	
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SHORTENED STATUTORY PERIOD OF RESPONSE			MAIL DATE	DELIVERY MODE
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Please find below and/or attached an Office communication concerning this application or proceeding.

If NO period for reply is specified above, the maximum statutory period will apply and will expire 6 MONTHS from the mailing date of this communication.

Office Action Summary

Application No.

09/502,133

Applicant(s)

HELSON, HAROLD E.

Examiner

Hugh Jones

Art Unit

2128

-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --

Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) OR THIRTY (30) DAYS, WHICHEVER IS LONGER, FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

Status

- 1) ☒ Responsive to communication(s) filed on 25 September 2006.
- 2a) ☐ This action is **FINAL**. 2b) ☒ This action is non-final.
- 3) ☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

Disposition of Claims

- 4) ☒ Claim(s) 1, 5, 9 and 13-27 is/are pending in the application.
- 4a) Of the above claim(s) _____ is/are withdrawn from consideration.
- 5) ☐ Claim(s) _____ is/are allowed.
- 6) ☒ Claim(s) 1, 5, 9, 13-27 is/are rejected.
- 7) ☐ Claim(s) _____ is/are objected to.
- 8) ☐ Claim(s) _____ are subject to restriction and/or election requirement.

Application Papers

- 9) ☐ The specification is objected to by the Examiner.
- 10) ☐ The drawing(s) filed on _____ is/are: a) ☐ accepted or b) ☐ objected to by the Examiner.
Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).
Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).
- 11) ☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

Priority under 35 U.S.C. § 119

- 12) ☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).
- a) ☐ All b) ☐ Some * c) ☐ None of:
- ☐ Certified copies of the priority documents have been received.
 - ☐ Certified copies of the priority documents have been received in Application No. _____.
 - ☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).
- * See the attached detailed Office action for a list of the certified copies not received.

Attachment(s)

- 1) ☒ Notice of References Cited (PTO-892)
- 2) ☐ Notice of Draftsperson's Patent Drawing Review (PTO-948)
- 3) ☒ Information Disclosure Statement(s) (PTO/SB/08)
Paper No(s)/Mail Date 9/25/2006.
- 4) ☐ Interview Summary (PTO-413)
Paper No(s)/Mail Date. _____.
- 5) ☐ Notice of Informal Patent Application
- 6) ☐ Other: _____.

DETAILED ACTION

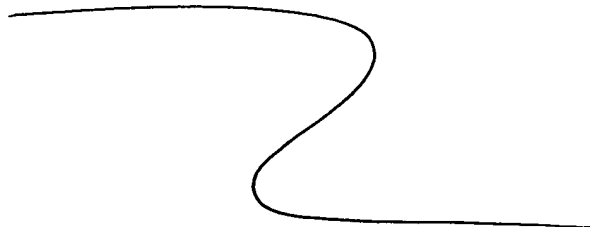
1. Claims 1, 5, 9, 13-27 of U. S. Patent 09/502,133 are in front of the office for consideration and remain pending.

Information Disclosure Statement

2. Applicants have submitted a lengthy information disclosure statements subsequent to the notice of allowance. This submission, coupled with the IDS's of record include close to two thousand pages of extremely dense and advanced chemistry. See MPEP section 2004 (Aids to Compliance With Duty of Disclosure) recites the following (emphasis added):

13. It is desirable to avoid the submission of long lists of documents if it can be avoided. Eliminate clearly irrelevant and marginally pertinent cumulative information. If a long list is submitted, **highlight those documents** which have been specifically brought to applicant's attention and/or are known to be of most significance. See Penn Yan Boats, Inc. v. Sea Lark Boats, Inc., 359 F. Supp. 948, 175 USPQ 260 (S.D. Fla. 1972), aff 'd, 479 F.2d 1338, 178 USPQ 577 (5th Cir. 1973), cert. denied, 414 U.S. 874 (1974). But cf. Molins PLC v. Textron Inc., 48 F.3d 1172, 33 USPQ2d 1823 (Fed. Cir. 1995).

3. Applicants have provided no guidance. Respectfully, the Examiner requests Applicant's technical assistance in reviewing said submissions. Applicant is qualified to provide said assistance for the following reasons: 1) Many of the references are referred to in the specification; and 2) Applicant is a leader in the field (as evidenced by publications and thesis).



Claim Rejections - 35 USC § 101

4. 35 U.S.C. 101 reads as follows:

Whoever invents or discovers any new and useful process, machine, manufacture, or composition of matter, or any new and useful improvement thereof, may obtain a patent therefor, subject to the conditions and requirements of this title.

5. **Claims 1, 5, 9, 13-27 are rejected under 35 U.S.C. 101 because the claimed invention is drawn to non-statutory subject matter since the claims do not produce a concrete, useful and tangible result.**

6. **Consider claim 1:**

1. (currently amended) A method for use in deriving a chemical structure diagram, comprising:

identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure;

~~representing wherein the instance of symmetry as a list of groups of~~ includes
symmetrically equivalent atoms and bonds;

~~expressing the instance of chemical structural symmetry a positioner positioning~~
symmetrically equivalent atoms and bonds in the chemical structure diagram in accordance with
the identified symmetry.

7. The claimed result in claim 1 is not tangible. The same reasoning holds true for all claims.

8. An invention which is eligible for patenting under 35 U.S.C. 101 is in the useful arts when it is a machine, manufacture, process or composition of matter, which produces a concrete, tangible, and useful result. *The fundamental test for patent eligibility is thus to determine whether the claimed invention produces a “useful, concrete and tangible result.”* The test for practical application as applied by the

examiner involves the determination of the following factors:

(1) Useful - The Supreme Court in *Diamond v. Diehr* requires that the examiner look at the claimed invention as a whole and compare any asserted utility with the claimed invention to determine whether the asserted utility is accomplished. Applying utility case law the examiner will note that:

(a) the utility need not be expressly recited in the claims, rather it may be inferred.

(b) if the utility is not asserted in the written description, then it must be well established.

9. Furthermore, although the claims are interpreted in light of the specification, limitations from the specification are not read into the claims. See *In re Van Geuns*, 988 F.2d 1181, 26 USPQ2d 1057 (Fed. Cir. 1993).

(2) Tangible - Applying *In re Warmerdam*, 33 F.3d 1354, 31 USPQ2d 1754 (Fed. Cir. 1994), the examiner will determine whether there is simply a mathematical construct claimed, such as a disembodied data structure and method of making it. If so, the claim involves no more than a manipulation of an abstract idea and therefore, is nonstatutory under 35 U.S.C. 101. In *Warmerdam* the abstract idea of a data structure became capable of producing a useful result when it was fixed in a tangible medium which enabled its functionality to be realized.

(3) Concrete - Another consideration is whether the invention produces a concrete result. Usually, this question arises when a result cannot be assured. An appropriate rejection under 35 U.S.C. 101 should be accompanied by a lack of

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enablement rejection, because the invention cannot operate as intended without undue experimentation.

Claim Rejections - 35 USC § 102

10. The following is a quotation of the appropriate paragraphs of 35 U.S.C. 102 that form the basis for the rejections under this section made in this Office action:

A person shall be entitled to a patent unless –

(b) the invention was patented or described in a printed publication in this or a foreign country or in public use or on sale in this country, more than one year prior to the date of application for patent in the United States.

11. Claims 1, 5, 9, 13-27 are rejected under 35 U.S.C. 102(b) as being clearly anticipated by Helson (The inventor's PhD thesis - of record).

12. The table of contents disclose:

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13. Helson discloses:

identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure (fig. 4.5; chapter 4; fig. 3.5, pg. 221, fig. 4.9, fig. 5.4);

wherein the instance of symmetry includes symmetrically equivalent atoms and bonds (page 246; fig. 4.5; chapter 4, fig. 4.9, 5.4);

a positioner positioning symmetrically equivalent atoms and bonds in the chemical structure diagram in accordance with the identified symmetry (page 246; fig. 4.5; chapter 3).

As for dependent claims, see pp. 169, 155-156, 173-212 (redrawing), 207-209, 227-230 (redrawing), table 4.3 (example of candidates); chapter 3 (redrawing) chapter 4 (examples of symmetry).

14. Also see:

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ISI	sym	Identification of Identical Structures
IVP	sym	Iterative Vertex Partitioning
MA	sym	Morgan algorithm
RSCT	SDG	Ring Symmetry Conversion Table
SDCO	sym	Symmetry-derived canonical order
SDG	SDG	Structure Diagram Generation (<i>q.v.</i>)
SP	sym	Symmetry Perception
SRAB	sym	Symmetry-Reduced A/B

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Connection Table The different connection tables used by CAMEO are:

- a) CSS. The ordinary structure storage format. Consists of a list of atoms, with coordinates, element type and charge, and bonds, with the atom pair forming the bond, order, and stereochemistry.
- b) CNAB. During translation of a chemical name (see Graphics chpt.) a simplified, compact CT is built up. Its principal omission is atom coordinates.
- c) Morgan Table. The Morgan table is a data structure similar to that used in the MA. It is used during the search for the canonical table.
- d) Canonical Connection Table (CCT). A highly encoded data structure similar to the Morgan Table in which the structures' A/B's have been canonically sequenced. It is possible to tell if two structures are identical or not by comparing their CCT's.

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Perception The process in which the A/B of a structure is examined to deduce higher level information, such as the presence and location of different element types (oxygen, silicon, etc.), rings, aromaticity, stereochemistry, symmetry, and the canonical connection table.

Perception-Derived Structure See *Derived Structure*

Perception Phase (Graphics) There are five distinct occasions when perception is performed: 1) sketch-time; 2) other graphics-time; 3) pre-mechanistic; 4) mechanistic; 5) post-mechanistic. All perception is channeled through one of two executives, PERCEP (pre- and post-mechanistic) and MCHPRCP (all others). Several flags control what sort of perception-induced alterations are permissible.

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Reposition (SDG) The final stage in *Structure Diagram Generation*, in which molecules are translated (shifted) to maximize the distance between them while maintaining their size as much as possible. Consists of two steps:

- a) Analytic placement.
- b) Dynamic repositioning. The fragments are treated as if they were charged particles that repel one another. They are allowed to move under each other's forces until they come to rest at equilibrium.

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Stereochemistry Most important stereochemistry of organic molecules can be represented in CAMEO, i.e. enantiomers and double bond stereoisomers. The notable omission is allene stereochemistry. A racemic mixture is represented by the absence of wedged or dotted bonds. Mixtures of *cis/trans* isomers are represented by labeling the double bond with a "U"; see Appendix B for a discussion. On rare occasions, usually in bridged ring systems, the program is unable to design a diagram in which a double bond has the correct *cis* or *trans* substituent pattern; an "I" is drawn beside such bonds to indicate that their stereochemistry is opposite that shown.

Structure One or more molecules that collectively constitute a chemical system undergoing reaction or emerging from reaction. The structure is a unit of storage; it is described by an A/B table, a tree node number, and more or less information about its role as a starting material and/or product.

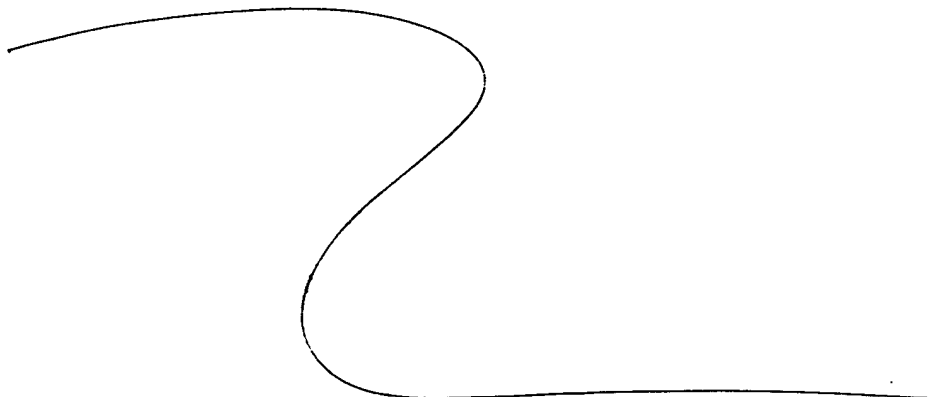
Structure Diagram Generation (SDG) The introduction or optimization of the two-dimensional coordinates in a connection table, especially for the purpose of realizing an aesthetic drawing. Consists of: a) Regularizing bond lengths and angles, and rendering rings in a conventional orientation. b) Redistributing molecules within the plotting area. Cf. *Reposition*.

Symmetry An object is symmetric if it contains components that are equivalent by some specified criteria. Equivalent components belong to the same "equivalence class," or "orbit." Frequently there are several orbits in one molecule, e.g. the two in butane.

Of the several types of chemical symmetry known, the one that reflects equivalent chemical reactivity is configurational symmetry.

Symmetry-Reduced A/B (SRAB) (Symmetry) The smallest subset of the A/B sufficient to reproduce the chemistry of the parent. In cyclohexane, for example, any one atom (bond) is representative of the entire molecule. Limiting attention to the SRAB saves computation time and avoids duplicate products due to symmetry. Reactions which involve more than one atom (bond), however, such as periodate oxidation of vicinal diols, may not rely upon the SRAB.

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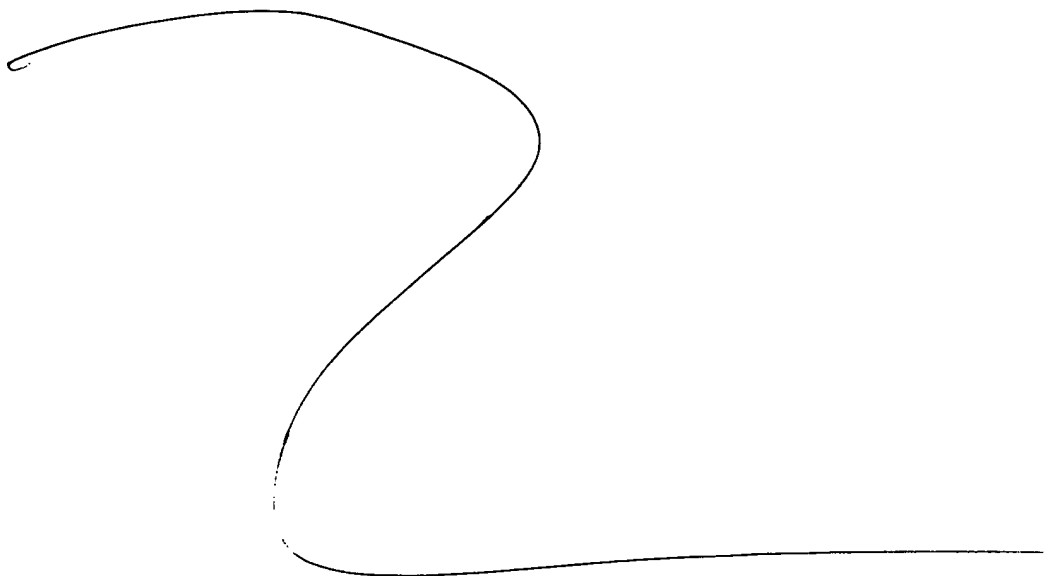
As has been seen, some approaches to isomorphism also yield symmetry, and vice versa. There is a fundamental reason why the two problems are related: a simple proof shows that they are formally equivalent; any method to solve one can be modified to solve the other.⁴ On a practical level they appear similar because some solutions to both involve partitioning or growing paths, resulting in overlap of these algorithms.

Placement in CAMEO

Before describing implementational details, it is shown how SP and ISI are situated within CAMEO. Fig. 4.4 highlights the overall program flow. Symmetry perception occurs during the middle of perception (whether graphic, mechanistic, pre- or post-mechanistic). CCT-coding occurs only at the end of pre- and post-mechanistic perception, i.e. once for the starting material and once for each product. Reaction intermediates may be perceived during the mechanistic phase but are not ordinarily CCT-coded. Because of this arrangement SP is needed and executed much more often than CCT-coding. It therefore made sense to develop an SP procedure that was fast on its own without concern for obtaining a CCT.

The symmetry algorithm requires stereochemical perception information, and must therefore reside after the point in the perception sequence where that is derived. CCT-coding could be performed at any time afterwards, and is performed at the end of a perception pass. Record is kept of which structures have been coded, so that ISI will merely check which structures are not coded, and codes them.

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Implementation of Symmetry Perception in CAMEO

The approach we have taken to symmetry perception is entirely original, as it was conceived and implemented without benefit of the literature. Upon review of the literature it is found to be similar to that published by Shelley and Munk more than a decade earlier,^{20,22} and that of Balaban *et al.* several years ago.^{6,2,2} The basic strategy is Iterative Vertex Partitioning (IVP), in which local molecular irregularities are propagated through the molecule until all atoms are partitioned into a stable number of distinct types. Because our implementation was conceived independently it is somewhat different. For one thing our symmetry perception has the extra responsibilities described in the previous section. For another, Shelley and Munk's algorithm, despite its suggestions, does not know what to do with stereochemistry or aromaticity, while Balaban *et al.*'s approach cannot treat stereochemistry at all without resorting to path-growing; our method treats these features routinely and rapidly. Finally, our algorithm is the first we know of not based on path growing to yield bond symmetry as well as atom symmetry.

fig. 4.5:

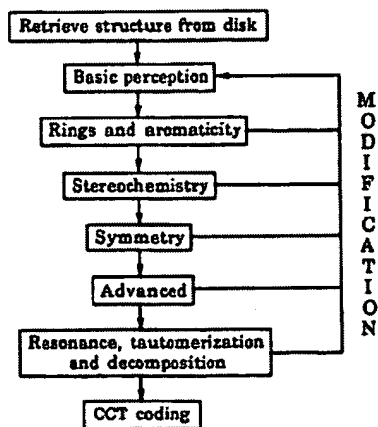


Figure 4.5. The perception phase

Fig. 4.9:



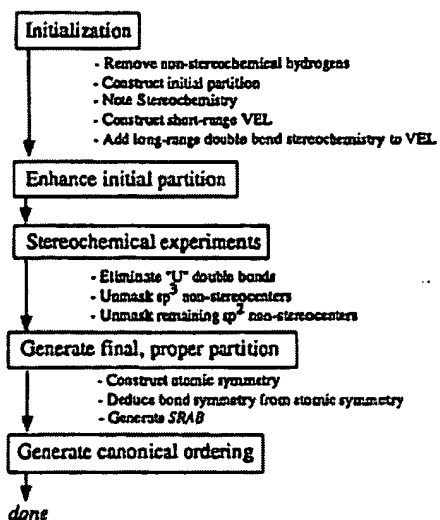


Figure 4.9. Symmetry perception

Table 4.3:

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Table 4.3. Symmetry perception timing information

Structure	No. Equivalence Classes: Atoms/Bonds ^a	Passes: Soft + Hard ^b	CPU ^c (10 ⁻² sec)
methane	1 / 0	0 + 0	0.1
ethane	1 / 1	1 + 1	0.3
propane	2 / 1	1 + 1	0.4
butane	2 / 2	1 + 1	0.7
decane	5 / 5	4 + 1	2.4
decanol	11 / 10	4 + 0	1.9
2-cyanonaphthalene	12 / 13	4 + 0	2.3
benzopyrene	5 / 6	3 + 1	8.3
adamantane	2 / 1	1 + 1	2.1
adamantan-1-ol	5 / 4	2 + 1	2.3
adamantan-2-ol	6 / 5	3 + 1	2.6
cubane	1 / 1	1 + 1	2.0
moebius cubane	1 / 1	1 + 1	2.0
moebius cubane ^d	1 / 2	7 + 3	6.1
cubanol	5 / 4	3 + 1	2.1
benzene	1 / 1	1 + 1	1.3
naphthalene	3 / 4	2 + 1	2.2
retinol	20 / 20	6 + 1	9.3
strychnine	25 / 31	3 + 0	6.4
morphine	25 / 29	2 + 0	6.0
muscarine	13 / 13	6 + 1	4.5
isoprene	5 / 4	1 + 0	0.5
2-methyl-2-butene	5 / 4	4 + 1	1.3
cyclohexene	3 / 4	4 + 1	1.7
1-methylcyclohexene	7 / 7	2 + 0	1.2
1,2-dimethyl-cyclohexene	4 / 5	3 + 1	2.3
2,2-dimethylpropane	2 / 1	1 + 1	0.8
glycerol	4 / 3	2 + 1	1.0
penicillanic acid	14 / 15	5 + 1	4.0
inositol	18 / 18	27 + 0	20.1
1-butene	4 / 3	1 + 0	0.4
cis-2-pentene	5 / 4	2 + 0	0.8
U-2-pentene	5 / 4	2 + 0	0.9
22 as drawn	24 / 25	11 + 2	19.1
racemic 22	18 / 19	5 + 1	11.2
3-methyl-tridecane	14 / 13	4 + 0	2.8
2-methyl-tridecane	13 / 12	6 + 1	3.8
7-methyl-tridecane	8 / 7	3 + 1	3.3

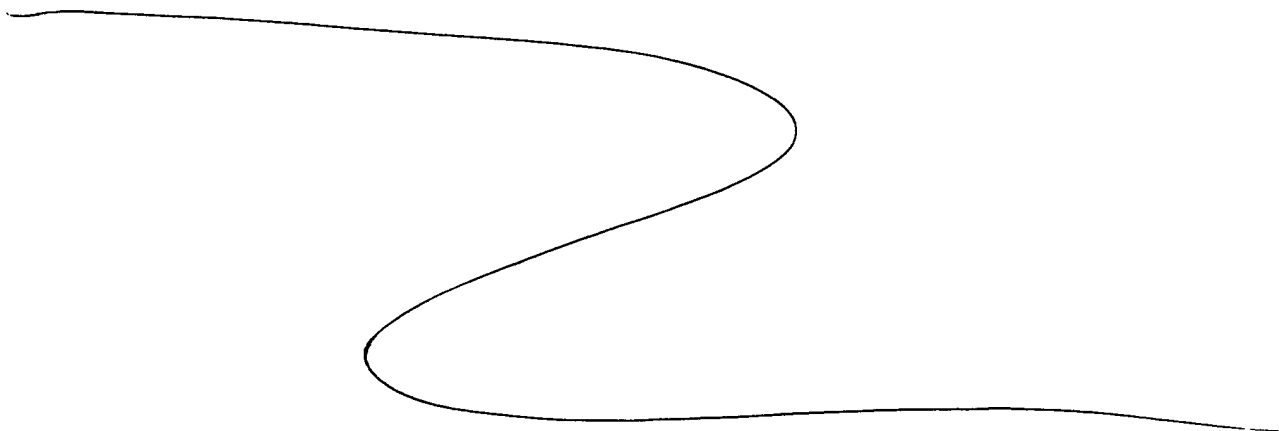
^aNote that the numbers increase with decreasing symmetry. An asymmetric molecule has an equivalence class for every one of its atoms and bonds.

^bStructures for which the number of hard passes is zero necessarily lack any (configurational) symmetry.

^cBy comparison, it took 499 sec to find the 9592 primes between 2 and 100,000, inclusive, factoring every odd number.

^dWith ring membership checks.

Fig. 5.4



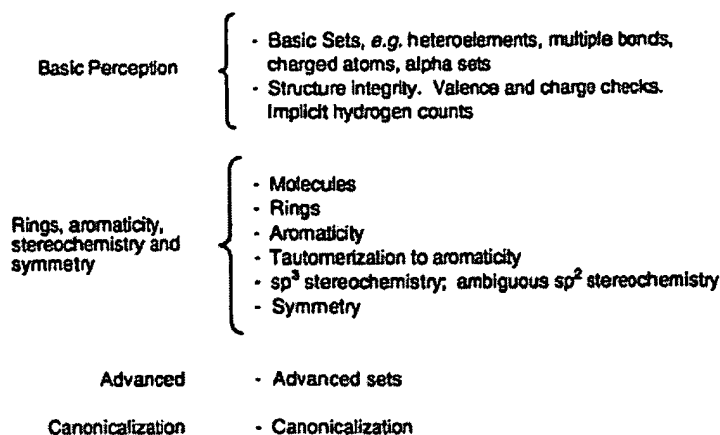


Figure 5.4. Components of the perception phase

Claim Rejections - 35 USC 103

15. The following is a quotation of 35 U.S.C. 103(a) which forms the basis for all obviousness rejections set forth in this Office action:

(a) A patent may not be obtained though the invention is not identically disclosed or described as set forth in section 102 of this title, if the differences between the subject matter sought to be patented and the prior art are such that the subject matter as a whole would have been obvious at the time the invention was made to a person having ordinary skill in the art to which said subject matter pertains. Patentability shall not be negated by the manner in which the invention was made.

16. Claims 1, 5, 9 are rejected under 35 U.S.C. 103(a) as being unpatentable over (Hu et al. or Shelley et al. or Fan) in view of Helson (thesis).

17. Hu et al. disclose computer perception of topological symmetry from a connection table (see abstract).

18. Shelley et al. also disclose computer perception of topological symmetry from a connection table (see pg. 247).

19. Fan et al. disclose detection of constitutionally equivalent atoms from a connection table (see page 654).
20. Hu et al. or Shelley et al. or Fan et al. do not expressly disclose positioning the atoms and bonds.
21. Helson discloses positioning in chapter 3 (cameo) of symmetrical structures (chapter 4).
22. It would have been obvious to one of ordinary skill in the art at the time of the invention to modify each base teaching with the secondary teaching because Helson discloses displaying positioning the atoms and bonds and its benefits, namely that disclosed in 1-5 of the thesis.
- 23. Claims 13-27 are rejected under 35 U.S.C. 103(a) as being unpatentable over (Hu et al. or Shelley et al. or Fan et al.) in view of Helson and in further view of (Chem 3D [of record] and Razinger et al. [of record]).**
24. Hu et al. or Shelley et al. or Fan et al. do not expressly disclose all *examples* of symmetry operations.
25. Chem3D discloses symmetry operations and properties and their manipulation in molecular modeling and analysis (chapters 4-5).
26. It would have been obvious to one of ordinary skill in the art at the time of the invention to modify the base teaching with the secondary teaching because Razinger et al. expressly discloses the importance of studying the various symmetries (first two paragraphs, col. 1, page 197) and carrying out and representing various chemical symmetry operations (chapter 4-5) when modeling and analyzing chemical structures.

Response to Arguments

27. Applicants have filed no arguments.

28. Any inquiry concerning this communication or earlier communications from the examiner should be:

directed to: Dr. Hugh Jones telephone number (571) 272-3781,

Monday-Thursday 0830 to 0700 ET,

or

the examiner's supervisor, Kamini Shah, telephone number (571) 272-2279.

Any inquiry of a general nature or relating to the status of this application should be directed to the Group receptionist, telephone number (703) 305-3900.

mailed to:

Commissioner of Patents and Trademarks

Washington, D.C. 20231

or faxed to:

(703) 308-9051 (for formal communications intended for entry)

or (703) 308-1396 (for informal or draft communications, please label *PROPOSED* or *DRAFT*).

Dr. Hugh Jones

Primary Patent Examiner

December 8, 2006


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TECHNOLOGY CENTER 2100